A New Monte Carlo Application for Complex Sample Geometries

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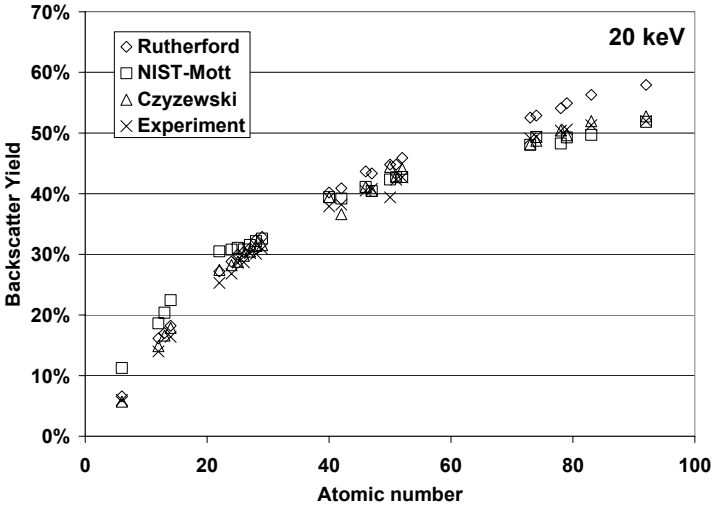
The CSTL research seeks to develop a library of Monte Carlo simulation routines capable of handling samples of arbitrary geometric complexity for performing quantitative microanalysis on micron-sized particles.

Performing quantitative microanalysis on micrometer-sized particles has always been a challenge. The volume of the particle is typically smaller than the electron beam excitation volume and x-ray absorption corrections are complicated by surface topology. Some researchers have approached this problem by approximating the particle as a simple geometric shape such as a cylinder, a rectangular, or triangular prism. While this approach is better than applying bulk correction methods, it may be possible to combine topological measurements from multiple imaging detectors to build a more accurate three-dimensional model of the unknown particle. This model could then become the input sample structure for a Monte Carlo simulation. The Monte Carlo simulation could be compared to Monte Carlo simulations of bulk references and the result could be iterated in a manner similar to the iterative correction processed used by the standard ZAF correction* scheme. The result is likely to be more accurate quantitative results. However, this scheme relies on the availability of a Monte Carlo model that can handle complex sample geometries. Our work seeks to develop a library of Monte Carlo simulation routines capable of handling samples of arbitrary geometric complexity.



The modeled backscatter yield for various different implementations of the electron elastic scattering cross-section compared with published measured values from Heinrich. Rutherford corresponds to a simple screened Rutherford cross-section; NIST-Mott and Czyzeweski are different implementations of the Mott cross-section. The Czyzewski cross-section reproduces the experimental results most accurately across the full range of atomic numbers.

We developed and tested a Monte Carlo simulation implemented in platform-independent Java code. We have evaluated various algorithms for electron elastic (see figure) and inelastic scattering cross section, electron energy loss, fluorescence yield and mass absorption coefficient. For each algorithm class, we selected the one that we determined produced the most realistic results. These algorithms have been implemented into a model in which the sample is represented by instances of a generic *Shape* interface. (*Shape* refers to a Java interface – a contract between a class's user and implementer). The *Shape* interface represents samples of arbitrary complexity with sufficient detail for the purposes of this model. Implementations of the *Shape* interface have been created for basic shapes such as spheres, blocks, and the volume defined by the intersection of an arbitrary number of directed planes. In addition, implementations of the *Shape* interface have been created to represent the union of two or more *Shape*s and the difference of two *Shape*s (the volume of *Shape* A minus the intersection between *Shape* A and *Shape* B). By combining these *Shape*s programmatically, samples of arbitrary complexity can be built from primitive *Shape*s.

Assigning particles to a descriptive class through quantitative microanalysis is hampered by morphologically induced particle-to-particle variance. We anticipate that by better modeling the shape of the particle we will be able to reduce particle-to-particle variance and thereby improve our ability to differentiate particles of similar but different materials. In the coming year, we plan to use the results from this Monte Carlo simulation to develop and evaluate more computationally efficient analytical expressions for quantifying particulate samples.

***ZAF Correction:** Conversion of the X-ray intensities to concentration based on measurement of the pure element intensities and composition of corrected factors for "atomic number effect" (Z), the "absorption correction" (A), and the "fluorescence correction" (F).